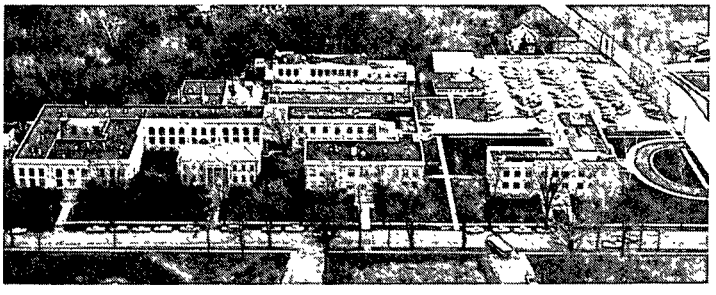


THE INSTITUTE OF PAPER CHEMISTRY, APPLETON, WISCONSIN

STATUS REPORT

To The

Project Advisory Committee

Systems Analysis

October 23-24, 1986
The Institute of Paper Chemistry
Continuing Education Center
Appleton, Wisconsin

NOTICE & DISCLAIMER

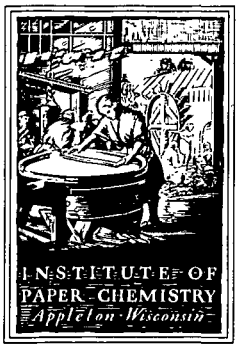
The Institute of Paper Chemistry (IPC) has provided a high standard of professional service and has exerted its best efforts within the time and funds available for this project. The information and conclusions are advisory and are intended only for the internal use by any company who may receive this report. Each company must decide for itself the best approach to solving any problems it may have and how, or whether, this reported information should be considered in its approach.

IPC does not recommend particular products, procedures, materials, or services. These are included only in the interest of completeness within a laboratory context and budgetary constraint. Actual products, procedures, materials, and services used may differ and are peculiar to the operations of each company.

In no event shall IPC or its employees and agents have any obligation or liability for damages, including, but not limited to, consequential damages, arising out of or in connection with any company's use of, or inability to use, the reported information. IPC provides no warranty or guaranty of results.

This information represents a review of on-going research for use by the Project Advisory Committees. The information is not intended to be a definitive progress report on any of the projects and should not be cited or referenced in any paper or correspondence external to your company.

Your advice and suggestions on any of the projects will be most welcome.



THE INSTITUTE OF PAPER CHEMISTRY
Post Office Box 1039
Appleton, Wisconsin 54912
Phone: 414/734-9251
Telex: 469289

September 22, 1986

TO: Members of the Systems Analysis Project Advisory Committee

Enclosed for your review is a brief status report for the process simulation work.

Our effort over the last reporting period has been devoted to developing the structure for performance attribute modeling and testing the combined optimization/simulation packages on a realistic problem. In addition to these two major efforts, we have also worked on improving the physical property routines available for MAPPS and developing some general purpose "utility" routines that can ease the construction of new process modules. Most of this development work will be incorporated in a new version to be released the latter part of this calendar year.

The meeting will be held in the Continuing Education Center, October 23 and 24. Rooms and meals will be available for those who wish to stay at the Center. You should have received the registration material which was mailed by Dr. Wahren's office on August 4. You may register by either returning the form which was enclosed with that mailing or by calling Mrs. Barbara Bisby (414/738-3328) by October 1. Members of the MAPPS Users Group will also be staying at the Center, so please get your reservation request to Barbara as soon as possible.

Sincerely,

Peter E. Parker
Group Leader
Process Modeling Group
Engineering Division

PEP/sjb
Enclosure

TABLE OF CONTENTS

PRELIMINARY AGENDA

SYSTEMS ANALYSIS PROJECT ADVISORY COMMITTEE MEETING

The Institute of Paper Chemistry
Continuing Education Center
Appleton, Wisconsin

Thursday, October 23, 1986

11:30-1:00	Lunch - CEC Dining Room	
1:00-5:00	PAC Meeting	
I.	Review of MAPPS' Status	Pete Parker
II.	Performance Attribute Modeling	Pete Parker
III.	Mechanical Pulping Models	Gary Jones
IV.	Utility Model Development	Mike Schreiter
V.	Optimization	Gary Jones
	A. Data Reconciliation	
	B. Process Design	
VI.	Future Developments	Pete Parker
5:00-6:30	Cocktails and Dinner	
7:00-?	MAPPS Users Group Meeting	

PRELIMINARY AGENDA (CONTD.)

SYSTEMS ANALYSIS PROJECT ADVISORY COMMITTEE MEETING

The Institute of Paper Chemistry
Continuing Education Center
Appleton, Wisconsin

Friday, October 24, 1986

This morning session will be devoted to discussing major "future work" issues. The main items are listed below, with more details provided in the status report. Of prime concern is your estimate of the priorities to be assigned to the various tasks.

7:00 a.m. Breakfast (CEC Dining Room)

8:00-10:00 PAC Meeting (small conference room, CEC)

I. Optimization

Importance

Make or Buy

Delivery Methodology

II. Product Performance Modeling

Importance

Need for Expert Systems

Manpower Commitment

8:30-12:00 MAPPS Users Group Meeting (large conference room, CEC)

PROJECT ADVISORY COMMITTEE - SYSTEMS ANALYSIS

Dr. James D. Rushton (Chairman) - 6/88*
Manager, Process Technology
Pulp and Paper Group
Bowater, Inc.
200 E. Camperdown Way
P. O. Box 1028
Greenville, SC 29602
(803) 271-7733

Mr. James L. Bonner - 6/89
Director of Information Systems
and Services
MacMillan Bloedel Inc.
P. O. Box 336
Pine Hill, AL 36769
(205) 963-4391

Mr. John G. Dekker - 6/89
Staff Engineer - Process
Corporate Engineering Services
Container Corporation of America
500 E. North Avenue
Carol Stream, IL 60188
(312) 260-6888

Dr. Matthew R. Gordon-Clark - 6/89
Chief Research Associate
Scott Paper Company
Scott Plaza
Philadelphia, PA 19113
(215) 521-5000

Dr. Edward G. Kelleher - 6/88
Director, Energy and Process
Engineering & Analytical Services
Champion International
West Nyack Road
West Nyack, NY 10994
(914) 578-7296

Dr. Ronald Mann - 6/89
Senior Process Engineer
James River Corporation
P. O. Box 19090
Green Bay, WI 54307-9090
(414) 499-0641

Mr. Ronald Montgomery - 6/87
Group Leader
Research & Development
Union Camp Corporation
P. O. Box 3301
Princeton, NJ 08540
(609) 896-1200

Dr. John Perry - 6/89
Group Leader
Electrical/Control Technology
Kimberly-Clark Corporation
2100 Winchester Road
Neenah, WI 54956
(414) 721-5182

Mr. Charles G. Rapp - 6/87
Research Associate
Corporate Research
Hammermill Paper Company
P. O. Box 10050
Erie, PA 16533
(814) 456-8811

Dr. Venki Venkatesh - 6/89
Consulting Engineer
The Mead Corporation
Courthouse Plaza, N.E.
Dayton, OH 45463
(513) 222-6323

Mr. W. Guyton Wilkinson - 6/88
Project Development
Stone Container Corporation
3805 Presidential Parkway
Suite 101
Atlanta, GA 30340
(404) 452-1321

* date of retirement
9/16/86

THE INSTITUTE OF PAPER CHEMISTRY

Appleton, Wisconsin

Status Report

to the

SYSTEMS ANALYSIS

PROJECT ADVISORY COMMITTEE

Project 3471

PROCESS MODELING AND SIMULATION

September 17, 1986

PROJECT SUMMARY FORM

DATE: September 17, 1986

PROJECT NO. 3471 - Process Modeling and Simulation

PROJECT LEADER: P. Parker

IPC GOAL:

To develop and support a marketable computer modeling capability to cover the full spectrum of mill types and problems of interest to Institute staff and member companies.

OBJECTIVE:

To develop and support the MAPPS simulation package.

CURRENT FISCAL YEAR BUDGET: $150,000

SUMMARY OF RESULTS SINCE LAST REPORT: (March, 1986 - September, 1986)

Version 2.0, modification level 1 was released in April, 1986.
System modified to incorporate performance attributes.
Mechanical pulping module development nearly completed.
Extensive test of optimization capability completed.

STATUS

Four more copies of MAPPS have been licensed since the last Project Advisory Committee meeting, bringing the total number of licensed copies to 23. With one exception, all of these users have been upgraded to Version 2.0, modification level 1 and support for the original release version, Version 1.0 has been dropped.

µMAPPS no longer runs with only 512 kB of memory. The current minimum size memory requirement is about 530 kB of user RAM, thus requiring a system with a minimum of 576 kB. With the next release, the minimum configuration will be a 640 kB microcomputer equipped with a numeric coprocessor chip. We are continuing to evaluate methods for avoiding the 640 kB limit of current IBM personal computer type hardware, but do not have an immediate solution. Solutions being considered are overlays, custom code configurations, and reduction of features.

We are actively working on release 3.0 of MAPPS. This new release, expected late this fall, will incorporate the mechanical pulping modules, the structure for performance attribute modeling, and several new physical property routines. We are currently testing the mainframe version of this code and will begin testing the personal computer version shortly. We expect this new version of µMAPPS to require a machine with 640 kB of memory.

The Users Group has been fairly active and has supplied the MAPPS group with the specification for a digester model that they would like to see developed for MAPPS. We are considering this specification and how best to implement it.

PERFORMANCE ATTRIBUTES

We have modified the structure of MAPPS to include arrays for handling performance attributes. For every defined material stream, there is a corresponding performance stream or PAS. The attributes of the PAS depend upon both the type of the associated material stream and user-specifed information. Default definitions of the PAS attributes are contained in a table similar to that for the material streams. In addition to the default definitions, there are several "extra" definitions that the user can use to redefine the default. For example, the PAPER type material stream will have a default PAS type of PAPER. However, the user can change the default definition of the PAS to, for example, STOCK with a simple command. However, unlike the material streams, the various attributes of a PAS may not be dynamically redefined. Table 1 lists the current attributes from which the PAS definitions are built.

Table 1. Performance attributes.

Number	Attribute
1	Number
2	Type
3	Kappa No.
4	Mean Fiber Length
5	Standard Deviation of Length
6	Mean Fiber Width
7	Standard Deviation of Width
8	K Factor
9	Canadian Standard Freeness
10	Adsorption Coefficient
11	Curl
12	Fiber Density
13	Fiber Tensile Strength
14	Fiber Modulus
15	Cell Wall Thickness

Many of the process modules will not modify the PAS information for its associated streams. To insure that attribute information is passed through the

process, the executive will assign inlet PAS information to the outlet PAS. We have developed a simple algorithm to process situations in which the number of inlet streams does not match the number of outlet streams. Figure 1 shows the basic information flow for the PAS information.

As can be seen from Table 1, MAPPS does not yet have an extensive list of performance attributes. The attributes contained in the table are used to support the attribute modeling contained in the mechanical pulping modules. These modules and their associated attributes are an initial attempt to incorporate attribute modeling in a material and energy balance package. As such, they serve as guidelines for future development effort by the MAPPS staff and the user community.

We recognized that modeling performance attributes was going to be a complex task. As we have developed the mechanical pulping modules and further explored the needs for performance attribute modeling, it has become reasonably evident that MAPPS, as it currently exists, may not be an appropriate tool for this work. Some attributes can be easily carried through the process; other attributes are the result of the totality of the process and modeling information is not yet available. Expert systems are an appropriate tool for much of this latter type of analysis. We are exploring the potential for combining the results of a MAPPS simulation with an expert system to predict the potential end-use performance.

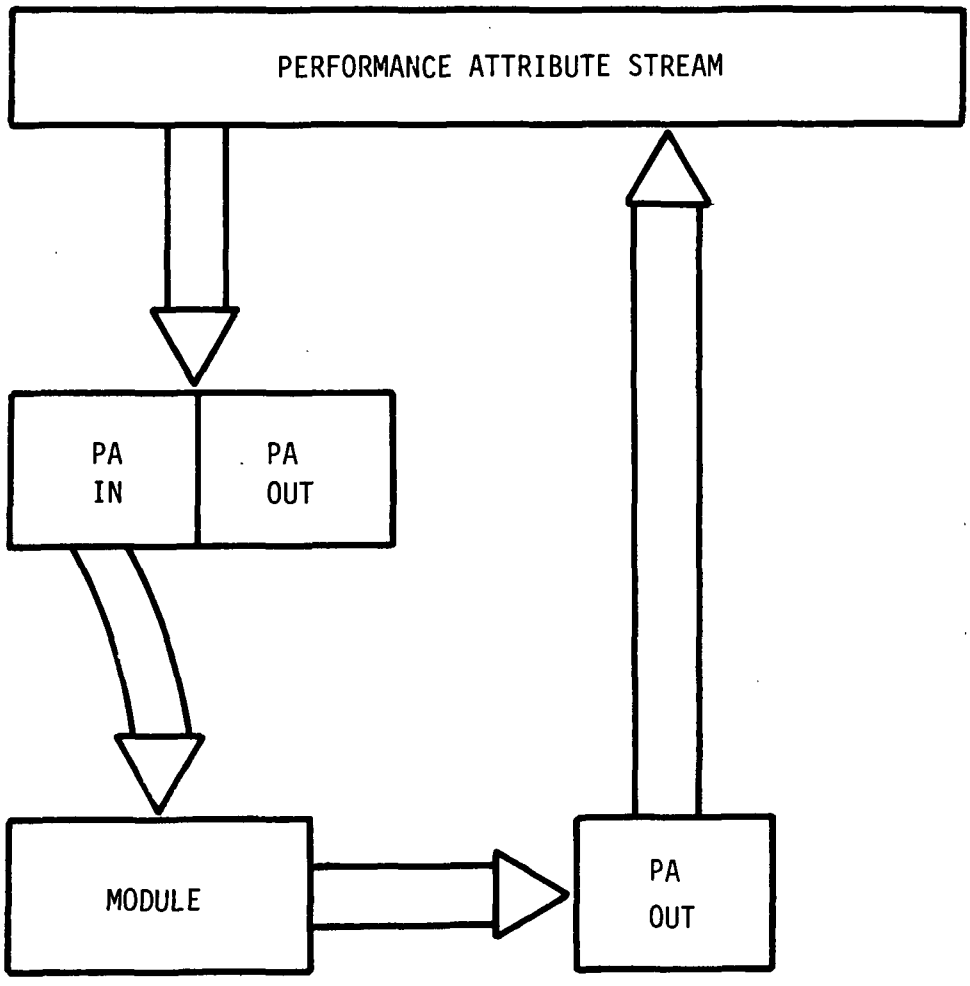


Figure 1. Performance attribute structure.

MECHANICAL PULPING

Four new mechanical pulping modules were developed which simulate the main features of mechanical pulping processes. The modules simulate refining of chips and fibers, mixing of fibers, separations with pressure screens, centricleaners, thickening and consistency control, and peroxide bleaching. Chemical and thermal pretreatment and latency aspects are not yet explicitly accounted for. However, these could be added later as additional modules or as additional features to existing modules. A mechanical pulping process flow sheet was developed to simulate converting chips into bleached pulp. The flow sheet shown in Fig. 2 includes the following process steps:

three refiners: chip, secondary and reject
primary screening
primary centricleaning
reject cleaning
reject centricleaning
thickeners for consistency control
stock mixing and recycle
single-stage peroxide bleaching

The key aspect of the new modules is their use of performance attributes or PATs in the simulation. We use PATs in the development of the mechanical pulping modules to primarily test the feasibility of using them generally throughout MAPPS.

Each stream in Fig. 2 now consists of the conventional stream data such as thermodynamic data and component flows plus a performance attribute substream containing PAT data.

Four of the PATs are statistical parameters which define the fiber length and width distributions. These are the mean and standard deviation of each distribution. All the mechanical pulping modules change the PATs. These

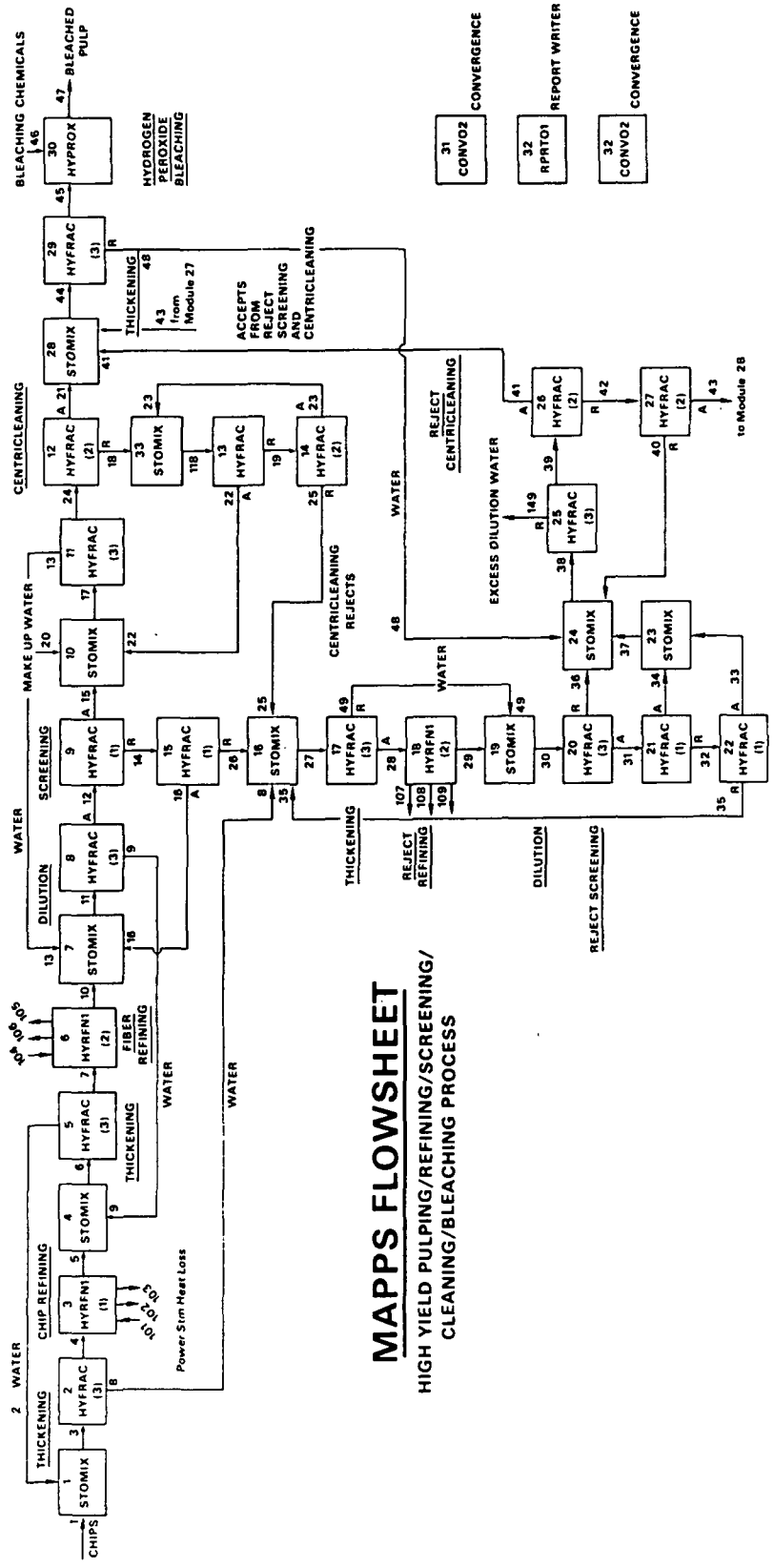


Figure 2. Mechanical pulping flow sheet.

in turn affect the flows of fibers in each stream. A fifth PAT, the absorption coefficient, is reduced during bleaching.

Performance attributes and conventional MAPPS variables are now used by new property models to predict pulp and handsheet properties such as Canadian Standard Freeness, wet-web strength, tensile and burst indices, breaking length, roughness, and tear.

MECHANICAL REFINING

The chip and fiber refiner modules are based on the statistical and kinetic work of Johnson, Yan, Corson, Irani, Epstein, and others. The fiber size distribution parameters of the inlet fiber stream are changed by the application of power to the refiner. The chip refiner converts chips with a given average length and width into an outlet fiber stream containing a range of smaller fibers, shives, and fines.

The fiber refiner converts an inlet fiber stream into an outlet fiber stream. In each case both the average length and width decrease and the distributions become narrower. The distribution parameters calculated by the module are placed in the PATs substream to be passed to another module.

Energy input for refining raises the temperature of the system. The result is steam formation and an increase in fiber consistency across the refiner.

Another PAT which changes during refining is the fiber specific surface area. The models of Strand and Edwards are used to predict the specific surface area parameter, K-factor, from the consistency and the specific power input. The specific surface is computed from a second model which includes the K-factor

and the fiber length distribution. There are models for both the primary and the secondary refiner. The K-factor is carried in the performance attribute substream to compute specific surface wherever it is needed.

The Canadian Standard Freeness is another PAT computed by the refiner. Freeness is related to the surface area development of the fibers, i.e., to the formation of fibrils. For the chip refiner, freeness decreases linearly with increasing specific power. For other modules, freeness is related to the change in the K-factor which reflects the change in specific surface area. The relationship was derived by combining the relationships for freeness and specific power and that for K-factor and specific power. Elimination of specific power yields a relationship between freeness and K-factor. This relationship is applied to modules where K-factor changes but there is no application of specific power such as in mixing and splitting. It is also applied to the secondary and reject refining steps where there is no relationship available. This relationship will require verification.

FIBER MIXING

Mixing of material and energy streams is normally a straightforward calculation. However, in the mechanical pulping process, we must mix performance attributes as well as materials. The difficulty is due to the fact that many of the PATs are not conserved quantities. However, fiber dimensions and surface area are conserved during mixing and splitting operations which makes it possible to mix some PATs based on fundamental principles.

Since freeness depends on K-factor which relates to specific surface, a conserved quantity, it is also possible to compute the mixture freeness.

All other mixture PATs, e.g., absorption coefficient, are equal to the weight average of the inlet values.

FIBER SEPARATIONS

The principles of fiber separation are complex and highly dependent on geometrical factors and fiber properties. Detailed accounting of fiber length and width distributions offers an advantage over less detailed models of the fibers in predicting separation efficiency. By introducing PATs it is possible to develop more powerful models of fiber separation processes.

Two types of fiber separations considered are screening and centricleaning. In screening, separation occurs primarily based on fiber length or width (for slotted screens). Centricleaners separate by a combination of specific gravity and specific surface area. These are also related to fiber length and width. The probability of rejecting a fiber depends on the total flow split and the length and width of the fiber. There are 100 different fiber dimensions represented internally, each with a different reject probability. The mass flows of the lumped fiber components in the streams are computed from the fiber separation efficiency and the fiber length and width distributions.

The performance attributes of the accept and reject streams are computed in the same fashion as for the mixer. The accept stream has fewer shives and more long fibers while the reject stream has more shives and shorter fibers. The PAT values will reflect the change in length, width, and specific surface area of the fibers. Although the models for the centricleaner and screen are different, the effects on the fiber splits are similar. The module computes the overall pulp split, i.e., ratio of reject to inlet fibers. It also allows the user to specify the downstream pressures.

CONSISTENCY CONTROL

Consistency is varied over a considerable range in the mechanical pulping flow sheet. Refining is usually done at relatively high consistency, i.e., 10 to 20%, bleaching at 10 to 14%, screening at 1 to 2%, and centricleaning at less than 1%. Consistency is controlled to desired levels in the flow sheet by use of mixing and thickening. The thickening process is approximated by splitting some water and dissolved components to the underflow to achieve the desired consistency in the overflow (accepts). All fibers appear in the accepts. The PATs of the accepts are the same as those of the inlet fiber stream. All PATs are zero in the reject water stream.

YIELD LOSS

There is as yet no yield loss in any of the above modules. This limits application of these modules to simulation of RMP, TMP, and SGW.

BLEACHING

A hydrogen peroxide bleaching module has also been implemented. Peroxide bleaches the fibers without significantly reducing lignin content. Chromophores in the lignin are oxidized by the peroxide to insoluble carboxylic acids. These are neutralized in alkaline solution. Most color bodies change to a colorless form when oxidized. Color body removal reduces the light absorption. The bleaching process is, therefore, measured by the reduction of the absorption coefficient, Ck, with bleaching time.

The bleaching model is based on the extensive work of S. Moldenius. The overall rate depends on absorption coefficient (order is 2.2), peroxide concentration (order is 0.67) and alkalinity (order is 0.23). The rate constant

has the usual Arrhenius dependence on temperature (activation energy = 45000 j/mole) but also a strong dependence on pulp consistency. This effect has not been explained in the literature and is unique to peroxide bleaching. In addition to the consistency effect, the rate constant also depends on the initial pH of the solution. The rate goes through a maximum with increasing initial pH. This is explained by the competition between chromophore elimination and chromophore formation with elimination dominating except at very high pH. It is known that darkening occurs rapidly if the pulp is left at high pH.

Peroxide is consumed in proportion to the change in absorption coefficient. The relationship is linear with a slope which depends on both consistency and initial pH.

Acid is formed as the reaction proceeds. pH declines as the acids are neutralized in alkaline solution. This pH calculation is based on simplified acid base equilibrium. It does not include the real system which contains sequestering agents, dissolved acids, salts, additives, etc.

The reactor is modeled as an adiabatic plug flow reactor. The rate is integrated along the length of the reactor to determine the values of Ck and concentrations at each increment. The outlet absorption coefficient is calculated and placed in the PAT substream.

The module also calculates the following properties: sheet density, tensile strength, roughness, scott bond index, and tear strength for handsheets made from bleached pulp. Properties are based on Moldenius' data.

The modules are designed to allow the user to enter a variety of module parameters which override the default values. This mechanism enables the user to specify the flow sheet for unique processing conditions.

DEVELOPMENT OF LATENT PULP PROPERTIES

Pulp fibers from the refiner contain residual stresses which cause the fibers to curl and become tangled into rolls, ribbons, and nodules. Fiber aggregates which are stored for significant periods above the wet lignin or wet hemicellulose softening temperatures and then cooled retain residual stresses. Hot disintegration allows the aggregates to untangle and the fibers to straighten. Under the right conditions, the fibers release their latent properties. After cooling, the fibers retain their latent properties. Cooling fibers while in contorted aggregates leads to latency being set into the fibers, i.e., inherent properties are lost. Latency removal depends on consistency, time, temperature, and shear history as well as the properties of the pulp itself and is therefore a rather complex kinetic process.

In the present models, it is assumed that latency has been removed. The properties reflect their full potential. However, a performance attribute to simulate latency, i.e., curl, has been provided. A model to relate stock storage conditions to curl and curl to fiber and paper properties must be developed before latency can be simulated.

PULP AND PAPER PROPERTIES

Unbleached Pulp and Paper

Frequently used pulp and paper properties are computed through the property interface and displayed as module parameters for the refiner, mixer, and

fractionator modules. Properties are based on data by Law and Garceau which were recorrelated to a form useful for MAPPS. The models predict bulk, wet-web strength, tear factor, burst factor, and breaking length according to TAPPI standards. The models are based on mixtures of hardwoods and softwoods with different levels of fine, medium length and long fibers. The fiber length distribution is divided into three ranges and the weight fraction fibers in each range is used in the models.

Bleached Paper Properties

Properties for bleached pulp from the hydrogen peroxide bleaching stage are based on work by S. Moldenius. Properties showed a significant cross correlation. Most of the properties were very similar in form to sheet density. Roughness showed an inverse response to density as expected. Moldenius noted a significant improvement in properties with higher peroxide charge, a condition he referred to as hyperperoxide bleaching. Properties also increased significantly with increasing initial pH. The pH effect was larger at higher peroxide charge. These factors are accounted for in the property models.

RESULTS

The flow sheet was run for a variety of fiber species and a range of specific power values, screen, and centricleaner flow splits, etc. Performance attributes and properties throughout the flow sheet reflected the changes in fiber length and width distributions and fiber specific surface. The values obtained appear reasonable and are in agreement with typical mechanical pulp properties.

Simulations were made to show how fiber distribution changes with increasing specific power to the chip refiner from 20 to 60 hp-day/ton. The

widest shives decrease continuously, the middle shive fraction goes through a maximum, and the narrowest shive fraction increases. The behavior of the fiber fractions is similar. The longer fibers are broken down into shorter fibers which go through a maximum. Fines continuously increase with increasing power.

CONCLUSIONS

The four new mechanical pulping modules can be configured into a MAPPS flow sheet to simulate a variety of high yield pulping processes.

Module parameters (default or user-specified) play the significant role of representing a variety of effects such as chemical and thermal pretreatment and species, whose effects are as yet poorly understood.

The heavy reliance on performance attributes in these modules demonstrates that this feature is feasible and should be developed further with MAPPS.

UTILITY MODEL DEVELOPMENT

THE PROPERTY INTERFACE

Since the release of version 2.0, MAPPS has been using an interface routine called PROPRT to handle most requests for physical and thermodynamic property calculations. PROPRT was implemented to replace THERMO and STEAM as the interface between process models and the physical and thermodynamic routines. The use of a PROPRT as a common interface simplifies the task of implementing new property routines into MAPPS. Our recent efforts have included the continuing development of new property routines. This discussion focuses on the use of the property interface and the routines that are now available or will be available with the next release of MAPPS.

PROPRT AND PROPIN, PROPOT

The interface PROPRT works with two very important arrays - PROPIN and PROPOT. PROPIN is used to pass data to the property routine and PROPOT is used to return calculated data. The arrays PROPIN and PROPOT are important because they will be the exclusive vehicles for transferring data to and from every property routine in MAPPS. In many cases, the property routine being called will expect the array PROPIN to have a defined MAPPS material stream structure. The data are read from the stream structure and the calculated values are returned in the PROPOT array, also usually in a MAPPS material stream structure. However, there is no restriction on the structure of these two arrays, and in some cases only one or two array positions are used.

THE PROPERTY ROUTINES

THERM1

THERM1 is the workhorse of the property routines. It is responsible for the calculation of all stream physical and thermodynamic data such as total flow, heat capacity, enthalpy, and exergy. THERM1 handles the job previously done by THERMO. THERMO is now no more than an interface itself, copying data to the PROPIN array and passing control to PROPRT. For this reason, THERMO is considered an obsolete routine - its use is being discouraged and it will eventually be phased out.

STEAM

Subroutine STEAM will continue to function as the routine responsible for calculating water/steam properties. STEAM is used by THERM1 when properties of a water stream are needed. The properties that can be calculated by STEAM are:

pressure
temperature
quality
specific volume
specific enthalpy
specific entropy
heat capacity

Calls to STEAM require only specific combinations of the properties listed above to define the state of the water stream. This is one example of PROPIN and PROPOT not passing a full MAPPS material stream definition to the calculating routine.

DENGAS

DENGAS will be available with the next release. It will compute the density of a gaseous stream based on the ideal gas.

DENLIQ

DENLIQ is used to compute the density of a liquid stream. It uses the subroutine STEAM to calculate water density at the given conditions, and then computes corrections based on the amounts of fibrous and nonfibrous materials and the composition of the nonfibrous material (organic or inorganic). The specific gravity of the nonfibrous portion of the stream is based on Han's work [Tappi 40(11)(1957)].

VISLIQ

VISLIQ is used to compute the viscosity of a liguid slurry in units of centipoise. The algorithm is valid only for low concentrations of suspended solids. Any MAPPS material stream except the gaseous type can be handled, although water streams must be mostly liquid (quality less than 0.01).

MASSFR

MASSFR is used to convert a material stream's flows from units of mass/time (lb/hr or kg/hr) to fractions of the total mass flow.

MOLEFR

MOLEFR is used to convert a material stream's flows from mass/time to mole fractions of the total molar flow.

PMOLWT

PMOLWT is used to return the molecular weight of a stream component.

UTILITY ROUTINES (TOOLS)

MAPPS also contains a growing library of utility routines (what we sometimes call "tools") that, in some cases, are intimately related to the property interface and property routines. The most notable of these is the

property interface PROPRT, itself a utility routine. Some of the other utility routines that relate to property routines are discussed below.

PHASE

PHASE is used to classify the components of a stream in the following categories:

dissolved or suspended
volatile or nonvolatile
fibrous or nonfibrous
organic or inorganic

PHASE is used often by process models representing equipment such as washers, screens, and flash tanks.

UCONSY

UCONSY is used to compute the percent consistency and the percent dissolved solids of a material stream. Within MAPPS, consistency is defined as the ratio of suspended material over total material.

STRMAN

STRMAN is a stream analysis routine that performs an elemental analysis of the stream's combined flow. The analysis is based on the 14 elements currently used in the MAPPS stream database. These 14 elements can combine to form all of the currently defined stream components. This utility routine will be useful for process models that require chemical reactions. It will be available in the next release version.

UCOPYI AND UCOPYO

These two routines are used to copy data into the PROPIN array (UCOPYI) from the stream arrays SN, SI, or SO, and to copy data from the PROPOT array (UCOPYO) to the SN and SO arrays. UCOPYI and UCOPYO are useful when calling a property or utility routine that requires a full material stream structure in the PROPIN array or returns the results as a full material stream structure in the PROPOT array.

OPTIMIZATION

Optimization refers to the process of improvement toward the best of all possible worlds. Once a process has been simulated with a process simulation package, the next logical step is to somehow "optimize" the flow sheet. Various applications of process optimization are in reconciling data from an existing process for the purpose of improving process operation and control, in specifying optimal processing conditions for a fixed design, and specifying both optimal design and operating conditions.

In optimization, a set of independent variables is determined so as to minimize an objective function, Y, made up of a combination of dependent and independent variables subject to a series of constraint relations (both equality and inequality) and bounds on the independent variables. A variety of techniques to determine the optimum are in use. The best technique depends on the nature of the process to be optimized.

Combining an optimization package with a process simulation tool such as MAPPS would enhance the use of MAPPS and provide a more useful result. For example, a MAPPS flow sheet of a mechanical pulping process could be "optimized" to determine the specific power to the refiners to minimize shives in the bleached pulp. The optimizer could also optimize pulp or paper properties.

Combining MAPPS with an optimization package requires (1) an interface to communicate between them, and (2) a variety of algorithms to choose between to determine the search for different types of problems.

In 1983, Ken Saffran developed a package known as OPTIM and linked an early version of MAPPS to it with a simple interface. Saffran demonstrated that

OPTIM would work with this early version of MAPPS by optimizing several difficult process flow sheets such as a kraft pulping and recovery process, a black liquor oxidiation flow sheet, and a brownstock washing system. He determined the best of three interfaces and the best two algorithms from the standpoint of robustness, CPU time, and accuracy of the answers obtained.

Figure 3 is a schematic of connections between OPTIM, MAPPS, and the interface.

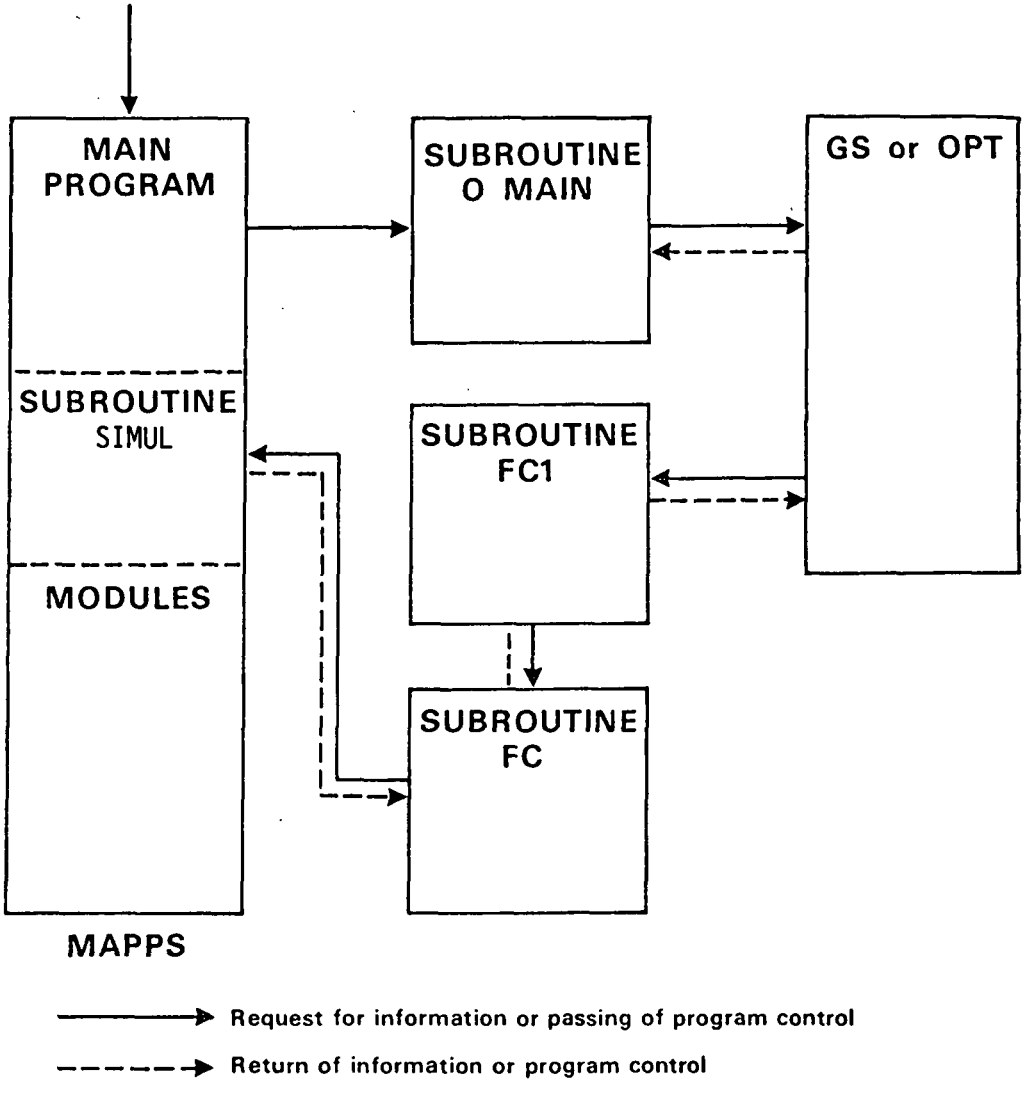


Figure 3. Simplified diagram of OPTIM with program control flows.

The user community has expressed an interest in having an optimization capability with the current version of MAPPS. In order to develop this new capability, we needed to determine whether OPTIM would be compatible with the present version of MAPPS and whether it would stand up to a truly difficult optimization problem.

The problem selected was a complex evaporator system shown in Fig. 4. The corresponding MAPPS flow sheet, shown in Fig. 5, employed the recently developed single-effect module (EVAP02) as well as flashes, heaters, heat exchangers, mixers, and splitters. The flow sheet was developed from industrial data and tested for sensitivity to variables such as weak liquor flows and concentration, steam flow and pressure, and evaporation dome pressures.

Because the process was an ongoing commercial system, the optimization problem was one of reconciling 52 measurements each with a different experimental error. The objective function for this type of problem is analogous to normal data regression. Y is equal to a weighted sum of squares of the differences between the data and the values calculated by MAPPS. The differences are normalized by the measurements. The weighting factors are inversely related to the experimental error for each measurement.

Data reconciliation for the evaporator system serves a variety of purposes: detecting faulty instruments, indirectly measuring scaling of the evaporator tubes, and providing guidance on the best boilout schedule. The evaporator system data was reconciled on a regular basis with MASSBAL, a process simulation package based on a simultaneous equation solving approach. MASSBAL attempts to satisfy the constraints while minimizing the objective function. In

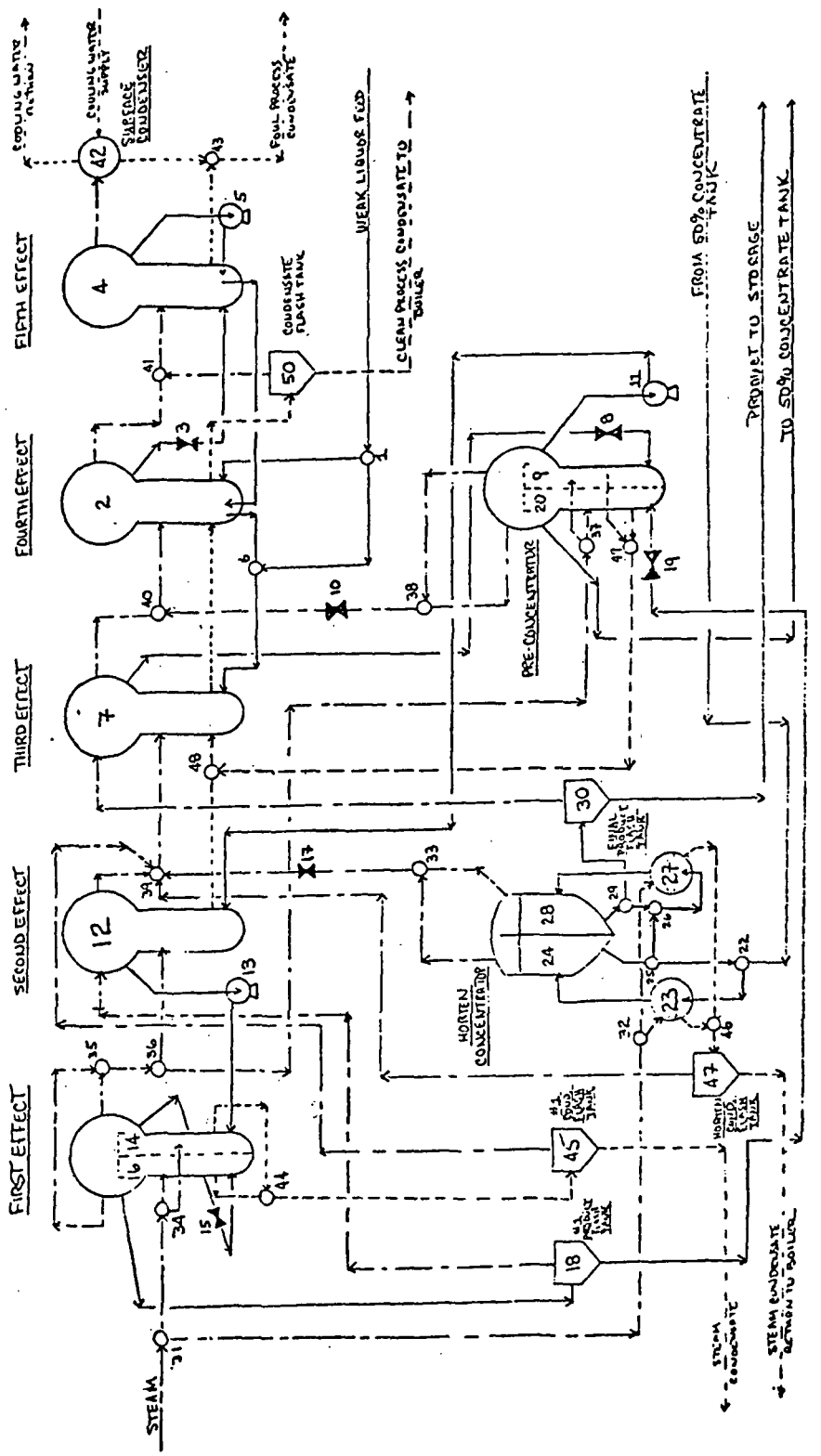


Figure 4. Black liquor evaporation process.

Figure 5. MAPPS flow sheet simulating black liquor evaporation process (see p. 25a).

the MAPPS approach, the constraints are satisfied iteratively each time the MAPPS flow sheet is converged.

There are a large number of constraints for this problem. Constraints include all of the mass and energy balances as well as physical constraints such as maximum black liquor solids concentrations and forbidding temperature crossover in the heat exchangers and evaporator. Fortunately, these are all automatically satisfied by MAPPS each time the flow sheet is converged.

The optimization begins with a converged MAPPS flow sheet at some set of conditions. The objective function is evaluated and the algorithm determines the changes in each variable to reduce Y. These are sent back to MAPPS which reconverges the flow sheet with the new values. The constraints are satisfied at this stage. OPTIM re-evaluates Y and determines a new search direction. The process is repeated until Y increases for an incremental change in any variable. The optimum is assumed. The MAPPS flow sheet at the optimum conditions and the values at each stage in the optimization are printed out.

OPTIM was compiled and linked to the current MAPPS code with minimal difficulty. The data to be reconciled was obtained and the data file was coded. These data were obtained on the system shown just prior to boilout. The weighting factors were selected based on assumed measurement accuracy. A subset of 36 variables was selected from the total of 52 used with MASSBAL. OPTIM was dimensioned to handle a maximum of 40 variables. However, the structure of MAPPS required that some variables had to be calculated in terms of other variables resulting in 36 variables for this problem. The remaining 16 variables, mainly intermediate liquor temperatures and concentrations, were calculated by MAPPS.

OPTIMIZATION RESULTS

Good agreement was obtained between the MAPPS optimization, the data, and the MASSBAL optimization. The values of the 36 optimized variables and the 16 calculated variables fell between the MASSBAL and the measured values. Optimization required on the order of 23 CPU minutes and 160 MAPPS simulations.

Differences between the MAPPS and MASSBAL values could be explained by the following differences in approach.

1. Steam superheat is lost at the evaporator inlet in MAPPS and at the outlet with MASSBAL.
2. Black liquor composition was not known. Although total solids was in agreement, heat capacity and enthalpy may have differed slightly.
3. Weighting factors used for the MASSBAL runs were not known.
4. The boiling point rise correlations may have differed.

The starting values for the optimization corresponded to conditions after boilout. The data which were reconciled corresponded to the day prior to boilout. At preboilout conditions the optimized steam flow rate and pressure were higher than the earlier conditions. The optimized heat transfer coefficients dropped in the high solids effects and increased in the low solids effects. This reflects the shift in load between the effects as scaling develops. The optimized MAPPS simulation results provided the information necessary to decide when to boilout the evaporator tubes.

DESIGN PROBLEM

Using the methods described above, a second problem was run with the MAPPS optimizer. The flow sheet was the mechanical pulping system shown in Fig.

2. The objective function was the sum of the flows of shives and fines in the bleached pulp and the independent variables were the specific power input to the chip, secondary, and reject refiners. At the values initially specified, 50, 40, and 20 hp-day/ton, respectively, total shives plus fines were equal to 150 lb/hr or 22.7% of the fiber fed.

Total shives plus fines were reduced to just 5.4 lb/hr or 0.8% at values of 47.7, 56.8, and 20.4 hp-day/ton after 83 iterations of OPTIM.

CONCLUSIONS

MAPPS can be used reliably with the appropriate optimization package. MAPPS is sufficiently robust to handle even difficult simulation optimization problems. It does not require excessive amounts of computer time to reach the solution.

A series of optimization algorithms should be developed specifically for MAPPS simulation. An improved interface in combination with new algorithms may be justified by reduced computation time.

MAPPS optimization appears feasible on the microcomputer although execution times may be excessive.